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Simulation of droplet spreading on porous substrates using smoothed particle hydrodynamics

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ABSTRACT

Small-scale fluid phenomena are being studied in many areas of engineering and research. This article focuses on small-scale droplet spreading and absorption on a porous substrate based on the SPH (Smoothed Particle Hydrodynamics) method. Three main factors that affect this process were considered: contact angle, pore sizes and gravity. Three various intrinsic contact angles, two different pore sizes with same porosity in comparison with flat surface and four different gravity conditions ($g = 0$ m/s^2 included) were applied to simulate the droplet spreading on porous substrates. The results show that the dependence of wetting region radius on time for both flat and porous substrates can be well divided into two spreading stages, i.e. a power-law inertial stage and viscous stage. To illustrate the counterbalance between droplet spreading and absorption, the evolution of liquid drop height was also examined, which indicates that the drop height decreases, while the wetting region radius increases as intrinsic contact angle decreases for both pore sizes. Besides that the effect of gravity on droplet spreading dynamics is also presented.

1. Introduction

Small-scale fluid phenomena are involved in various applications and research areas. Understanding the wetting behavior of droplet spreading on porous substrate is important for many industrious applications and scientific research, such as paper coating, printing and macroscopic flow phenomena like the spreading of gravity currents over porous beds [1]. Generally, this phenomenon is controlled by two main competitive processes, which are the droplet spreading on a textured surface and the imbibition inside the bulk porous media [9]. Both experiment and numerical methods were adopted to study the two competitive processes of sessile droplet wetting dynamics. Chen and Wang [5] studied water drop impact on different wood surfaces based experimental ways. Starov et al. [21] experimentally investigated the spreading of small silicone oil drops over various dry thick porous substrates, where the spreading process was divided into the first spreading step over the texture surfaces and the second imbibition step of droplets into the porous bulk. The drop base reaches its maximum quickly in the first step and then shrinks in the second step. Davis and Hocking [7,8] developed models based on lubrication theory to study the evolution time of drops, the position of contact line and the motion inside the porous media. Raiskinmäki [20] carried out three-dimensional simulations to study the effect of impact velocity and surface roughness on the spreading of droplets into a substrate consisting of randomly placed and orientated, freely penetrating disks using the lattice-Boltzmann method. Clark et al. [6] combined penetration equations with droplet spreading equations to describe the droplet spreading on porous surfaces. Alleborn and Raszillier [1] developed a spreading model based on Darcy's law. Frank and Perré [10] simulated the pore-level droplet spreading on porous surface using the lattice Boltzmann method.

Meshfree methods have been applied to simulate water flow in porous media. Ovaysi and Piri [19] developed a dynamic particle-based model for direct pore-level modeling of incompressible viscous fluid flow in disordered porous media. Tartakovsky et al. [24,23] developed a phenomenological Langevin model to simulate flow and multicomponent transport in porous media based on SPH (Smoothed Particle Hydrodynamics) method, however, the spreading was not included.

This paper presents the simulation of pore-scale droplet spreading on porous media using the SPH method. Better free surface tracking and large deformation solving, the advantage of SPH

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method makes it more suitable for this droplet-spreading problem. The surface tension is implemented using particle–particle interactions according to Tartakovsky and Meakin [22]. In this approach the ratio of fluid–fluid to solid–fluid forces controls the wetting behavior, such that different static contact angles were simulated and quantified. The capability of SPH method applied to small-scale liquid phenomena involved wetting behavior has been approved.

2. Formulation of SPH method

2.1. SPH fundamentals

In the SPH method, the fluid field can be represented by a set of particles with individual properties such as density and velocity. The fundamental principle [13,14,2,11,16] allows to approximate the function $A(\vec{r})$ in the following forms:

$$\langle A(\vec{r})\rangle = \int A(\vec{r}')W(\vec{r}-\vec{r}',h)d\vec{r}', \tag{1}$$

where h is the smoothing length and $W(\vec{r}-\vec{r}',h)$ is the weighting function or kernel function. For simplicity we drop the angle brackets to denote the approximation in the following. In discrete form, the function $A(\vec{r})$ can be approximated by the summation over all the particles within the compact region by the kernel function as follows,

$$A(\vec{r}) = \sum_b m_b \frac{A_b}{\rho_b} W_{ab}, \tag{2}$$

where m_b and ρ_b are the mass and the density of particles respectively. $W_{ab} = W(\vec{r}_a - \vec{r}_b, h)$ is the weight function or namely kernel. Among various types of kernel functions, this simulation is based on a quintic spline kernel [25],

$$W(r,h) = \alpha_D\left(1-\frac{q}{2}\right)^4(2q+1), \quad 0 \leqslant q \leqslant 2, \tag{3}$$

where $q = \frac{r}{h}$, α_D is $\frac{7}{4\pi h^2}$ in 2D and $\frac{21}{16\pi h^3}$ in 3D.

The derivative of the function can be calculated by

$$\frac{dA}{d\vec{r}} = \sum_b m_b \frac{A_b}{\rho_b}\vec{\nabla}_a W_{ab}, \tag{4}$$

where $\vec{\nabla}_a W_{ab}$ is the derivative of weighting or kernel function.

2.2. Basic SPH equations

The Navier–Stokes equations can be discretized using the SPH formalism to simulate the movement and the change of hydrodynamic features of particles. The Navier–Stokes equations with laminar viscous stresses are given by

$$\frac{d\rho}{dt} = -\rho\nabla\cdot v, \tag{5}$$

$$\frac{D\vec{v}}{Dt} = -\frac{1}{\rho}\vec{\nabla}P + \vec{g} + v_0\nabla^2\vec{v}. \tag{6}$$

Based on the fundamental principles mentioned in the previous section, Monaghan [14,15] presented an SPH discretization NS equations, where the laminar stress is given by Lo and Shao [26] as

$$(v_0\nabla^2\vec{v})_a = \sum_b m_b\left(\frac{4v_0\vec{r}_{ab}\vec{\nabla}_a W_{ab}}{(\rho_a+\rho_b)|\vec{r}_{ab}|}\right)\vec{v}_{ab}, \tag{7}$$

where v_0 is the kinetic viscosity of laminar flow. Then the continuity equation and momentum equation can be given by,

$$\frac{d\rho_a}{dt} = \sum_b m_b\vec{v}_{ab}\vec{\nabla}_a W_{ab}, \tag{8}$$

$$\frac{d\vec{v}_a}{dt} = -\sum_b m_b\left(\frac{P_b}{\rho_b^2}+\frac{P_a}{\rho_a^2}\right)\vec{\nabla}_a W_{ab} + \vec{g} + \sum_b m_b\left(\frac{4v_0\vec{r}_{ab}\vec{\nabla}_a W_{ab}}{(\rho_a+\rho_b)|\vec{r}_{ab}|}\right)\vec{v}_{ab}. \tag{9}$$

Assuming weakly compressible flow in SPH method, the state equation can be used and allows a faster determination of fluid pressure than solving Poisson's equation. Assuming a weakly compressible fluid Monaghan [12] employed an equation of state in the follow form:

$$P = B\left[\left(\frac{\rho}{\rho_0}\right)^\gamma - 1\right], \tag{10}$$

where $\gamma = 7$, $B = \frac{c_0^2\rho_0}{\gamma}$, $\rho_0 = 1000\ \mathrm{kg\ m^{-3}}$ the reference density and $c_0 = c(\rho_0) = \sqrt{\left(\frac{\partial P}{\partial\rho}\right)\Big|_{\rho_0}}$ is the speed of sound at the reference density. The speed of sound is 1 m/s in this simulation greater than ten times of maximum droplet velocity in order to describe the weakly compressible flow. The repulsive boundary condition is applied to this simulation and the Lennard-Jones force was used [15].

$$Fr_{ij} = \begin{cases} c_1\left[\left(\frac{dx}{r}\right)^{c_2} - \left(\frac{dx}{r}\right)^{c_3}\right]\frac{\vec{r}}{r^2}, & |r_j - r_i| \leqslant dx \\ 0, & |r_j - r_i| > dx, \end{cases} \tag{11}$$

where $c_1 = 0.5\,gH$, $c_2 = 12$, $c_3 = 6$ and dx is initial distance between two particles. H is determined according to the simulation dimension.

2.3. Surface tension model

Surface tension plays an important role in droplet spreading on flat surfaces and porous substrates. Morris [17] first applied the color function to the SPH method in order to simulate surface tension of the free surface flows and between fluids. However, this method is not applicable to create the surface tension between fluids with large density and viscosity ratio and can not simulate the force between fluid and solid and thus create a contact angle. Nugent and Posch [18] applied SPH method to a van der Waals fluid to examine the oscillation of droplets. Tartakovsky and Meakin [22] improved the SPH model, adding the fluid–fluid and fluid–solid particle–particle interactions, by defining the interaction force as

$$F_{ij} = \begin{cases} s_{ij}\cos\left(\frac{1.5\pi}{3h}|r_j - r_i|\right)\frac{r_j - r_i}{|r_j - r_i|}, & |r_j - r_i| \leqslant h \\ 0, & |r_j - r_i| > h, \end{cases} \tag{12}$$

where s_{ij} is the strength coefficient of the particle–particle interaction. The momentum equation with surface tension is given as follows:

$$\frac{d\vec{v}_a}{dt} = -\sum_b m_b\left(\frac{P_b}{\rho_b^2}+\frac{P_a}{\rho_a^2}\right)\vec{\nabla}_a W_{ab} + \vec{g} + \sum_b m_b\left(\frac{4v_0\vec{r}_{ab}\vec{\nabla}_a W_{ab}}{(\rho_a+\rho_b)|\vec{r}_{ab}|}\right)\vec{v}_{ab} + \frac{F_{ij}}{m_a}. \tag{13}$$

The effect of different contact angles can be simulated by defining different interaction coefficients s_{ij} between fluid and solid particles.

3. Results and discussion

3.1. Droplet dynamics

Fig. 1 shows the evolution of a single water droplet consisting of particles with the initial shape of cube. The momentum equation with surface tension Eq. (11) was used, and the simulation result